

LA-UR-21-23800

Approved for public release; distribution is unlimited.

Title: MD Simulations of Full-Scale HIV-1 Lipid Envelope on LANL Grizzly Supercomputer

Author(s): Bryer, Alexander
Reddy, Tyler John Edward
Lyman, Edward
Perilla, Juan Roberto

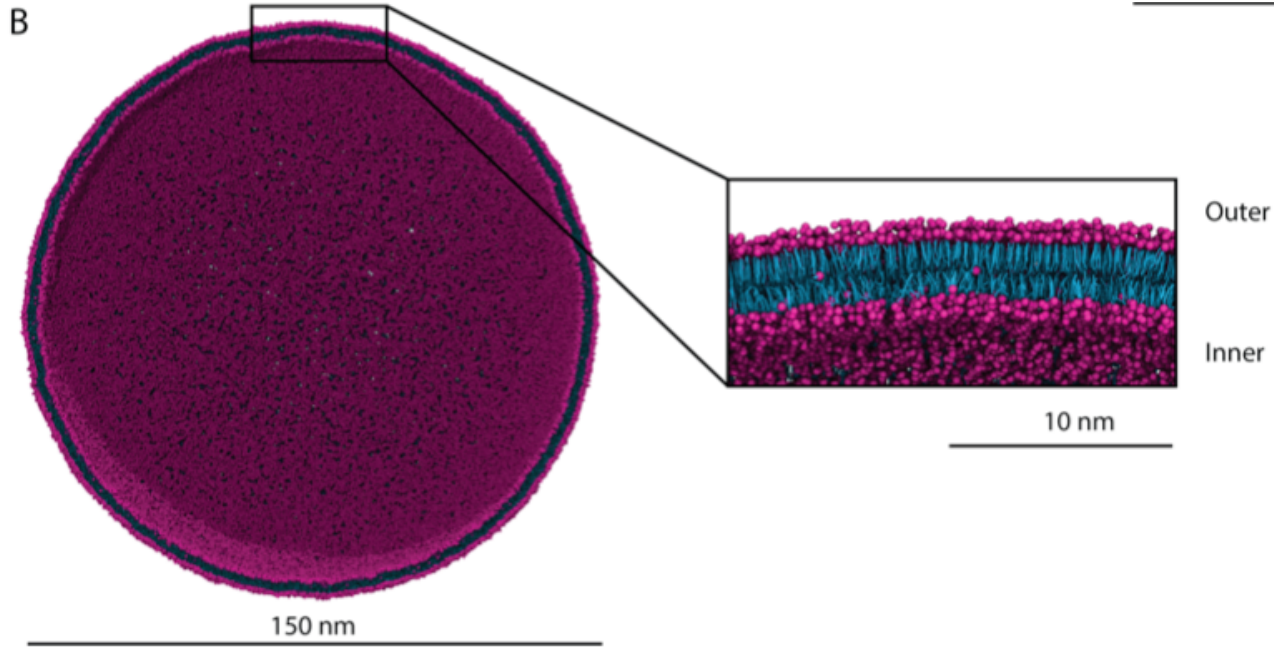
Intended for: Report

Issued: 2021-04-20

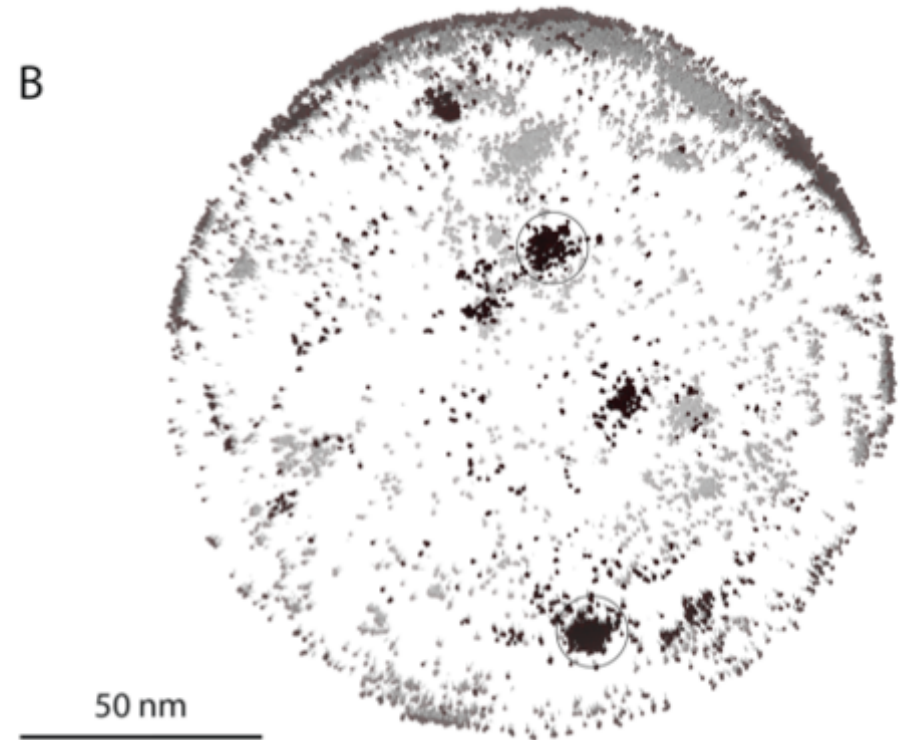
Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

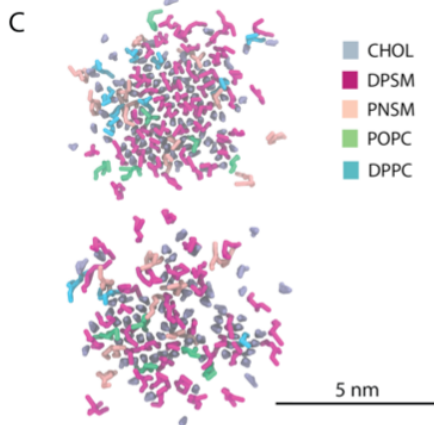
MD Simulations of Full-Scale HIV-1 Lipid Envelope on LANL Grizzly Supercomputer



Cross-section view of the HIV-1 vesicle after 5 microseconds of simulation with the MARTINI force field.



Determination of low-mobility regions in HIV-1 vesicle (circled) over the course of the simulation.



Identification of Lipid Species
In Low Mobility Regions

Results Submitted to: *ACS Central Science* in April 2021
Bryer, Alexander; Reddy, Tyler; Lyman, Edward; Perilla, Juan